Solving Expensive Environmental Engineering Problems with GORBIT

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We introduce a new global optimization algorithm, GORBIT for solving general simulation-based problems

$$\min \{f(x) : x \in \mathcal{D} \subset \mathbb{R}^n\}, \tag{1}$$

when $f(x) = F(x, S(x))$ depends on the output of a deterministic computer simulation S. The simulators of interest to us are expensive to evaluate because they involve numerically solving systems of partial differential equations governing the underlying physical phenomena. Due to this expense, the number of function evaluations available for solving (1) is limited by a computational budget. These simulators rarely provide the derivative $\nabla_x S(x)$ and computational noise often limits the accuracy to which the problem can be solved. Local solvers can get trapped in local minima where the function value is considerably larger than the global solution.

To address this complicated problem, we developed the GORBIT global optimization algorithm for bound-constrained domains $\mathcal{D}$. GORBIT is a two-stage algorithm, consisting of an exploration phase, in which the domain is sampled globally, and a refinement phase, where a local optimizer is employed. Based on its effectiveness in unconstrained local optimization, the derivative-free solver ORBIT [3] is used in the refinement phase. ORBIT relies on a trust-region framework and builds radial basis function models interpolating the function f at points where f has been evaluated. We introduce a multistart method MIPE (Maximum Information from Previous Evaluations), sharing some features with Multi Level Single Linkage (MLSL) [1], so that the global exploration phase can take advantage of the output from the local optimization runs. Modifications are made to ORBIT, such as accounting for bound constraints and using the information from the function values obtained during the global exploration phase in MLSL or MIPE.

GORBIT differs from existing multistart-based algorithms such as [2] in that it seeks to use as much of its own evaluation history as possible. We motivate the application of GORBIT on a bioremediation problem in which we wish to find a cost-effective treatment plan (consisting of pumping rates and well locations) to clean up contamination at the Umatilla Chemical Depot in Oregon.

References

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